

Sebastian Johann Wetzel

Employment

- 3/2025– **Founder**, *Maindframe - The Automated Lecture Project*, Automating lectures to bring customized education to every corner of the world., <https://maindframe.com/>
- 3/2023– **AI Advisor/ML Research Engineer**, *Homes Plus Magazine Inc.* / *University of Waterloo*, Research and development of an artificial intelligence + blockchain-powered real estate web platform, deployment of my own regression algorithm "Twin Neural Network regression" to real estate.
- 10/2019– **Research Scientist**, *Perimeter Institute*, Research at the intersection between theoretical physics and artificial intelligence
- 03/2025
- 5/2018– **Research Scientist**, *University of Heidelberg*, Research at the intersection between theoretical physics and artificial intelligence
- 7/2019

Education

PhD

- est. 2025 **PhD under special regulations in Computer Science**, *University of Cambridge*
- 05/2014– **PhD in Physics**, *University of Heidelberg*
- 05/2018

Master

- 10/2011– **Master of Science in Physics**, *University of Heidelberg*
- 01/2014
- 10/2010– **Master of Advanced Study in Applied Mathematics**, *University of Cambridge*, *Wolfson College*
- 06/2011

Bachelor

- 10/2007– **Bachelor of Science in Physics**, *University of Heidelberg*
- 08/2010

High School

- 06/2006 **Abitur**, *Hellenstein-Gymnasium Heidenheim*

Academic Contributions

Most Important Scientific Contributions

Proposal of unsupervised neural network-based frameworks for the calculation of phase diagrams which are now widely used to calculate phase diagrams in experimental and theoretical physics and material science.

Pioneering of interpretation of artificial neural networks in physics for artificial scientific discovery.

Pioneering of artificial intelligence in high energy lattice physics

Proposal of neural network-based variational approach to finding conserved quantities and symmetry invariants

Invention of twin neural network regression, likely the most versatile and accurate semi-supervised regression framework that combines consistency conditions, error estimates, ensemble generation, and adaptation to dynamically changing data. The algorithm is already employed by at least two companies.

Invention of symbolic gradients framework for the closed-form interpretation of any single neuron within artificial neural networks and thereby providing a solution to one variant of the neural network black-box problem.

Publications

An updated list can be found at

<https://scholar.google.de/citations?user=V0xTqc4AAAAJ>

Interpretable Machine Learning in Physics: A Review, *SJ Wetzel, R Iten, S Ha, M Klopotek, Z Liu*, arXiv preprint arXiv:2409.05305

Closed-Form Interpretation of Neural Network Latent Spaces with Symbolic Gradients, *Z Patel, SJ Wetzel*, arXiv preprint arXiv:2409.05305

Closed-Form Interpretation of Neural Network Classifiers with Symbolic Gradients, *SJ Wetzel*, Machine Learning: Science and Technology 6 (1), 015035

Twin neural network improved k-nearest neighbor regression, *SJ Wetzel*, International Journal of Data Science and Analytics, 1-11

How to get the most out of Twinned Regression Methods, *SJ Wetzel*, arXiv preprint arXiv:2301.01383

Unsupervised learning of Rydberg atom array phase diagram with Siamese neural networks, *Z Patel, E Merali, SJ Wetzel*, New Journal of Physics 24 (11), 113021

Modern applications of machine learning in quantum sciences, *A Dawid, J Arnold, B Requena, A Gresch, M Plodzien, K Donatella, K A Nicoli, P Stornati, R Koch, M Buettner, R Okula, G Munoz-Gil, R A Vargas-Hernandez, A Cervera-Lierta, J Carrasquilla, V Dunjko, M Gabriele, P Huembeli, E v Nieuwenburg, F Vicentini, L Wang, SJ Wetzel, G Carleo, E Greplova, R Krems, F Marquardt, M Tomza, M Lewenstein, A Dauphin*, arXiv preprint arXiv:2204.04198

Twin Neural Network Regression is a Semi-Supervised Regression Algorithm, *SJ Wetzel, RG Melko, I Tamblyn*, Machine Learning: Science and Technology 3 (4), 045007

Toward Orbital-Free Density Functional Theory with Small Data Sets and Deep Learning, *K Ryczko, SJ Wetzel, RG Melko, I Tamblyn*, Journal of Chemical Theory and Computation 18 (2), 1122-1128

Twin Neural Network Regression, *SJ Wetzel, K Ryczko, RG Melko, I Tamblyn*, Applied AI Letters 3 (4), e78

Spectral reconstruction with deep neural networks, *Lukas Kades, Jan M Pawłowski, Alexander Rothkopf, Manuel Scherzer, Julian M Urban, Sebastian J Wetzel, Nicolas Wink, Felix PG Ziegler*, Physical Review D 102 (9), 096001

Logic guided genetic algorithms, *D Ashok, J Scott, SJ Wetzel, M Panju, V Ganesh*, Proceedings of the AAAI Conference on Artificial Intelligence 35 (18), 15753

Discovering symmetry invariants and conserved quantities by interpreting siamese neural networks, *SJ Wetzel, RG Melko, J Scott, M Panju, V Ganesh*, Physical Review Research 2 (3), 033499

Exploring the Hubbard Model on the Square Lattice at Zero Temperature with a Bosonized Functional Renormalization Approach, *SJ Wetzel*, arXiv:1712.04297

Machine learning of explicit order parameters: from the Ising model to SU(2) lattice gauge theory, *SJ Wetzel, MScherzer*, Physical Review B 96 (18), 184410

Unsupervised learning of phase transitions: from principal component analysis to variational autoencoders, *SJ Wetzel*, Phys. Rev. E 96, 022140

Physics and the choice of regulators in functional renormalisation group flows, *JM Pawłowski, MM Scherer, R Schmidt, SJ Wetzel*, Annals of Physics 384, 165-197

Teaching

05/13-05/23, 2024 **Block Course at Triumph, (Virtual) Vancouver**, Large Language Models from Scratch

04/29-05/8, 2024 **Block Course at University of Waterloo/Perimeter Institute, (Virtual) Waterloo**, Large Language Models from Scratch

09/11-09/15, 2023 **Lecture at DKPI Summer School, Oberaichwald**, Introduction to Machine Learning

10/2013– **Supervisor**, for *Internship and Master Students*, including main supervision of:

Claudia Zendejas-Morales, 05/2023–, PSI Start

Ali Sarear Toosi, 12/2022–12/2024, PSI Masters

Zurab Jashi, 05/2022–12/2022, PSI Start

Zakaria Patel, 01/2021–11/2022, Internship

10/2012–07/2019 **Teaching assistant**, for *lectures in classical mechanics, analytical mechanics, statistical physics, quantum mechanics, advanced mathematics for physicists and for a student seminar in quantum mechanics*

Invited Conferences Presentations, Seminar Talks and Expert Panels

10-31-2023 **Flatiron Institute Seminar, New York**, Talk: Machine Learning of Conserved Quantities and Symmetry Invariants

06-15-2023 **Machine Learning for Quantum Many-Body Systems, Waterloo**, Talk: Machine Learning of Conserved Quantities and Symmetry Invariants

- 03-02-2023 **Machine Learning Approaches in Lattice QCD - an interdisciplinary exchange**, *Munich*, Talk: Physical Concepts from Neural Networks with two Inputs
Invited Panel Discussion for ML for Phase Transitions
Invited Panel Discussion for Interpretable ML in physics
- 09-22-2022 **Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology**, *Hamburg*, Talk: Revealing Physical Concepts Learned by Artificial Neural Networks
Invited Panel Discussion
- 09-27-2021 **Machine Learning for High Energy Physics, on and off the Lattice**, *Trento*, Talk: Interpreting Artificial Neural Networks in the Context of Theoretical Physics
- 08-27-2021 **Summer School: Machine Learning in Quantum Physics and Chemistry**, *Warsaw*, Talk: Challenging Traditional Beliefs in Machine Learning
- 06-30-2021 **Artificial Scientific Discovery**, (*Virtual*) *Erlangen*, Talk: Interpreting Artificial Neural Networks in the Context of Theoretical Physics
Invited Panel Discussion
- 06-16-2021 **Mila Seminar**, (*Virtual*) *Montréal*, Talk: Interpreting Artificial Neural Networks in the Context of Theoretical Physics
- 06-08-2021 **Canadian Association of Physicists Congress**, (*Virtual*), Talk: Interpreting Artificial Neural Networks in the Context of Theoretical Physics
- 12-02-2020 **Machine Learning Club**, (*Virtual*) *CEA Saclay, Johns Hopkins, IAC, Paris Observatory, UC Santa Cruz*, Talk: Siamese Neural Networks Learn Symmetry Invariants and Conserved Quantities
- 10-24-2019 **University of Waterloo Physics Seminar**, *Waterloo*, Talk: Machine Learning Phase Diagrams of the Ising Model and SU(2) Lattice Gauge Theory
- 11-05-2019 **First French-German Meeting in Physics, Mathematics and Artificial Intelligence Theory**, *Paris*, Talk: Can we trust phase diagrams produced by artificial neural networks?
- 04-11-2019 **Perimeter Institute Seminar**, *Waterloo*, Talk: Can we trust phase diagrams produced by artificial neural networks?
- 06-22-2018 **Optimising, Renormalising, Evolving and Quantising Tensor Networks**, *Dresden*, Talk: Exploring Phase Diagrams with Artificial Neural Networks
- 05-03-2018 **Isoquant Workshop**, *Heidelberg*, Talk: Exploring Phase Diagrams with Artificial Neural Networks
- 02-02-2018 **Institute for Applied Physics, Seminar**, *Tübingen*, Talk: Exploring Phase Diagrams with Artificial Neural Networks
- 10-04-2017 **9th Bethe Center Workshop**, *Bad Honnef*, Talk: Exploring Phase Diagrams with Artificial Neural Networks
- [Contributed Talks and Posters](#)
- 02-13-2019 **Machine Learning for Quantum Many-body Physics**, *Santa Barbara*, Poster: Exploring Phase Diagrams with Artificial Neural Networks
- 06-28-2018 **Machine Learning for Quantum Many-body Physics**, *Dresden*, Poster: Exploring Phase Diagrams with Artificial Neural Networks

- 03-20-2018 **Beyond Digital Computing**, *Heidelberg*, Poster: Interpretable Neural Networks for Learning Phase Diagrams
- 09-19-2016 **Exact Renormalization Group Conference**, *Trieste*, Poster: Physics and the Choice of Regulators in Functional Renormalization Group Flows
- 10-03-2015 **IMPRS-QD Annual Excursion**, *Neunkirchen*, Talk: Hubbard Model on the Square Lattice at Zero Temperature
- 02-03-2015 **HGSFP Winter School**, *Obergurgl*, Poster: Hubbard Model on the Square Lattice at Zero Temperature
- 09-24-2014 **Exact Renormalization Group Conference**, *Lefkada*, Talk: Competing Order Parameters and Multicritical Phenomena
- 07-02-2014 **FOR 723 Workshop**, *Wien*, Talk: Competing Order Parameters and Multicritical Phenomena

[Reviewer for Journals](#)

Journal of Chemical Physics

Physical Review B

Physical Review E

Physical Review Research

Physical Review Letters

European Physical Journal B

Physics of Fluids

Progress of Theoretical and Experimental Physics

Nature Computational Science

[Reviewer for Startup Incubators](#)

Creative Destruction Lab

--- Languages

German	Native
English	Fluent
French	Intermediate

--- Computing

Programming	C++, Python
Machine Learning	Tensorflow, Keras, PyTorch, Scikit-Learn
Internet	html, php, css
Blockchain	Solidity
Algebra	Mathematica

--- Scholarships and Awards

04/2009- Scholarship of the **German Academic Scholarship Foundation**. (Studienstiftung
01/2014 des deutschen Volkes)
10/2008- **Exemption from Tuition Fees** for excellent grades in university exams.
08/2010